

Sebacic acid, isobutyl 3-oxobut-2-yl ester

Inchi:	InChI=1S/C18H32O5/c1-14(2)13-22-17(20)11-9-7-5-6-8-10-12-18(21)23-16(4)15(3)19/h
InchiKey:	SMQVSQKGXHMWOI-UHFFFAOYSA-N
Formula:	C18H32O5
SMILES:	CC(=O)C(C)OC(=O)CCCCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]:	328.44

Physical Properties

Property code	Value	Unit	Source
gf	-500.96	kJ/mol	Joback Method
hf	-1027.59	kJ/mol	Joback Method
hfus	42.50	kJ/mol	Joback Method
hvap	79.94	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.827		Crippen Method
mcvol	280.930	ml/mol	McGowan Method
pc	1298.60	kPa	Joback Method
rinpola	2220.00		NIST Webbook
tb	816.81	K	Joback Method
tc	1007.05	K	Joback Method
tf	456.87	K	Joback Method
vc	1.085	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	873.36	J/molxK	816.81	Joback Method
cpg	889.61	J/molxK	848.52	Joback Method
cpg	904.82	J/molxK	880.22	Joback Method
cpg	919.00	J/molxK	911.93	Joback Method
cpg	932.16	J/molxK	943.64	Joback Method
cpg	944.33	J/molxK	975.34	Joback Method
cpg	955.50	J/molxK	1007.05	Joback Method
dvisc	0.0010953	Paxs	456.87	Joback Method
dvisc	0.0005029	Paxs	516.86	Joback Method

dvisc	0.0002715	Paxs	576.85	Joback Method
dvisc	0.0001646	Paxs	636.84	Joback Method
dvisc	0.0001088	Paxs	696.83	Joback Method
dvisc	0.0000768	Paxs	756.82	Joback Method
dvisc	0.0000570	Paxs	816.81	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355774&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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